Serdar Durdagi

List of Publications by Year
in descending order

167 papers	3,857 citations	117453 34 h-index	182168 51 g-index
184 all docs	184 docs citations	184 times ranked	4599 citing authors

#	Article	IF	Citations
1	Discovery of potent carbonic anhydrase and acetylcholine esterase inhibitors: Novel sulfamoylcarbamates and sulfamides derived from acetophenones. Bioorganic and Medicinal Chemistry, 2015, 23, 3592-3602.	1.4	137
2	Acetylcholinesterase and carbonic anhydrase inhibitory properties of novel urea and sulfamide derivatives incorporating dopaminergic 2-aminotetralin scaffolds. Bioorganic and Medicinal Chemistry, 2016, 24, 2318-2329.	1.4	131
3	Carbonic anhydrase inhibitory properties of novel benzylsulfamides using molecular modeling and experimental studies. Bioorganic Chemistry, 2014, 56, 75-82.	2.0	113
4	Kinetic and docking studies of phenol-based inhibitors of carbonic anhydrase isoforms I, II, IX and XII evidence a new binding mode within the enzyme active site. Bioorganic and Medicinal Chemistry, 2011, 19, 1381-1389.	1.4	97
5	Identification of Novel Cholesterol-binding Regions in Kir2 Channels. Journal of Biological Chemistry, 2013, 288, 31154-31164.	1.6	95
6	Computational design of novel fullerene analogues as potential HIV-1 PR inhibitors: Analysis of the binding interactions between fullerene inhibitors and HIV-1 PR residues using 3D QSAR, molecular docking and molecular dynamics simulations. Bioorganic and Medicinal Chemistry, 2008, 16, 9957-9974.	1.4	93
7	Combined Receptor and Ligand-Based Approach to the Universal Pharmacophore Model Development for Studies of Drug Blockade to the hERG1 Pore Domain. Journal of Chemical Information and Modeling, 2011, 51, 463-474.	2.5	88
8	Inhibition of acetylcholinesterase and butyrylcholinesterase with uracil derivatives: kinetic and computational studies. Journal of Enzyme Inhibition and Medicinal Chemistry, 2019, 34, 429-437.	2.5	76
9	Combinatorial peptide library screening for discovery of diverse Î±-glucosidase inhibitors using molecular dynamics simulations and binary QSAR models. Journal of Biomolecular Structure and Dynamics, 2019, 37, 726-740.	2.0	74
10	Modeling of Open, Closed, and Open-Inactivated States of the hERG1 Channel: Structural Mechanisms of the State-Dependent Drug Binding. Journal of Chemical Information and Modeling, 2012, 52, 2760-2774.	2.5	68
11	Nanoscale enzyme inhibitors: Fullerenes inhibit carbonic anhydrase by occluding the active site entrance. Bioorganic and Medicinal Chemistry, 2010, 18, 2822-2828.	1.4	66
12	The synthesis of novel sulfamides derived from Î²-benzylphenethylamines as acetylcholinesterase, butyrylcholinesterase and carbonic anhydrase enzymes inhibitors. Bioorganic Chemistry, 2017, 74, 238-250.	2.0	64
13	3D QSAR CoMFA/CoMSIA, molecular docking and molecular dynamics studies of fullerene-based HIV-1 PR inhibitors. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 6283-6289.	1.0	60
14	Development of accurate binding affinity predictions of novel renin inhibitors through molecular docking studies. Journal of Molecular Graphics and Modelling, 2010, 29, 425-435.	1.3	56
15	Structureâ€“activity relationships for the interaction of 5,10-dihydroindeno[1,2-b]indole derivatives with human and bovine carbonic anhydrase isoforms I, II, III, IV and VI. European Journal of Medicinal Chemistry, 2012, 49, 68-73.	2.6	54
16	Does the donorâ€“acceptor concept work for designing synthetic metals?. Journal of Molecular Modeling, 2006, 12, 687-701.	0.8	52
17	In Silico Drug Screening Approach for the Design of Magic Bullets: A Successful Example with Anti-HIV Fullerene Derivatized Amino Acids. Journal of Chemical Information and Modeling, 2009, 49, 1139-1143.	2.5	52
18	Synthesis, biological activity and multiscale molecular modeling studies of bis-coumarins as selective carbonic anhydrase IX and XII inhibitors with effective cytotoxicity against hepatocellular carcinoma. Bioorganic Chemistry, 2019, 87, 838-850.	2.0	49

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19	Design, synthesis and biological evaluation of novel nitroaromatic compounds as potent glutathione reductase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 5398-5402.	1.0	48
20	The Application of 3D-QSAR Studies for Novel Cannabinoid Ligands Substituted at the C1â€˜ Position of the Alkyl Side Chain on the Structural Requirements for Binding to Cannabinoid Receptors CB1 and CB2. Journal of Medicinal Chemistry, 2007, 50, 2875-2885.	2.9	47
21	Structural refinement of the hERG1 pore and voltageâ€sensing domains with ROSETTAâ€membrane and molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2922-2934.	1.5	47
22	Binding of novel fullerene inhibitors to HIV-1 protease: insight through molecular dynamics and molecular mechanics Poissonâ€“Boltzmann surface area calculations. Journal of Computer-Aided Molecular Design, 2011, 25, 959-976.	1.3	45
23	Binding Interactions of Dopamine and Apomorphine in D2High and D2Low States of Human Dopamine D2 Receptor Using Computational and Experimental Techniques. ACS Chemical Neuroscience, 2016, 7, 185-195.	1.7	45
24	Synthesis, anticholinesterase activity and molecular modeling study of novel carbamate-substituted thymol/carvacrol derivatives. Bioorganic and Medicinal Chemistry, 2017, 25, 1352-1363.	1.4	45
25	Application of 3D QSAR CoMFA/CoMSIA and in silico docking studies on novel renin inhibitors against cardiovascular diseases. European Journal of Medicinal Chemistry, 2009, 44, 3703-3711.	2.6	44
26	Virtual screening of eighteen million compounds against dengue virus: Combined molecular docking and molecular dynamics simulations study. Journal of Molecular Graphics and Modelling, 2016, 66, 99-107.	1.3	42
27	Investigating the molecular mechanism of staphylococcal DNA gyrase inhibitors: A combined ligand-based and structure-based resources pipeline. Journal of Molecular Graphics and Modelling, 2018, 85, 122-129.	1.3	42
28	Interaction of carbonic anhydrase isozymes I, II, and IX with some pyridine and phenol hydrazinecarbothioamide derivatives. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 5636-5641.	1.0	41
29	Investigation of Inhibition Mechanism of Chemokine Receptor CCR5 by Micro-second Molecular Dynamics Simulations. Scientific Reports, 2015, 5, 13180.	1.6	40
30	Antihypertensive Drug Valsartan in Solution and at the AT₁ Receptor: Conformational Analysis, Dynamic NMR Spectroscopy, in Silico Docking, and Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2009, 49, 726-739.	2.5	39
31	Inhibition of human carbonic anhydrase isozymes I, II and VI with a series of bisphenol, methoxy and bromophenol compounds. Journal of Enzyme Inhibition and Medicinal Chemistry, 2012, 27, 467-475.	2.5	39
32	Carbonic anhydrase inhibitors: Design, synthesis, kinetic, docking and molecular dynamics analysis of novel glycine and phenylalanine sulfonamide derivatives. Bioorganic and Medicinal Chemistry, 2015, 23, 7353-7358.	1.4	39
33	Characterization, in Vivo Evaluation, and Molecular Modeling of Different Propofolâ€“Cyclodextrin Complexes To Assess Their Drug Delivery Potential at the Bloodâ€“Brain Barrier Level. Journal of Chemical Information and Modeling, 2016, 56, 1914-1922.	2.5	39
34	Synthesis of Some Novel Norborneneâ€Fused Pyridazines as Potent Inhibitors of Carbonic Anhydrase and Acetylcholinesterase. Journal of Heterocyclic Chemistry, 2016, 53, 2049-2056.	1.4	39
35	Cholesterol up-regulates neuronal G protein-gated inwardly rectifying potassium (GIRK) channel activity in the hippocampus. Journal of Biological Chemistry, 2017, 292, 6135-6147.	1.6	37
36	Insights into the molecular basis of action of the AT1 antagonist losartan using a combined NMR spectroscopy and computational approach. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 1031-1046.	1.4	35

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37	Effects of propolis, caffeic acid phenethyl ester, and pollen on renal injury in hypertensive rat: An experimental and theoretical approach. Cell Biochemistry and Function, 2017, 35, 304-314.	1.4	35
38	Inhibition of mammalian carbonic anhydrases I-XIV with grayanotoxin III: solution and in silico studies. Journal of Enzyme Inhibition and Medicinal Chemistry, 2014, 29, 469-475.	2.5	33
39	Proposing Novel MAO-B Hit Inhibitors Using Multidimensional Molecular Modeling Approaches and Application of Binary QSAR Models for Prediction of Their Therapeutic Activity, Pharmacokinetic and Toxicity Properties. ACS Chemical Neuroscience, 2018, 9, 1768-1782.	1.7	33
40	Effects of Cholesterol on GPCR Function: Insights from Computational and Experimental Studies. Advances in Experimental Medicine and Biology, 2019, 1135, 89-103.	0.8	32
41	A computational study on cannabinoid receptors and potent bioactive cannabinoid ligands: homology modeling, docking, de novo drug design and molecular dynamics analysis. Molecular Diversity, 2010, 14, 257-276.	2.1	31
42	The discovery of new potent non-peptide Angiotensin II AT1 receptor blockers: A concise synthesis, molecular docking studies and biological evaluation ofÂN-substituted 5-butylimidazole derivatives. European Journal of Medicinal Chemistry, 2012, 55, 358-374.	2.6	31
43	Fullerene-based inhibitors of HIV-1 protease. Journal of Peptide Science, 2015, 21, 862-870.	0.8	31
44	Role of the pH in state-dependent blockade of hERG currents. Scientific Reports, 2016, 6, 32536.	1.6	31
45	Combined 3D QSAR and molecular docking studies to reveal novel cannabinoid ligands with optimum binding activity. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 6754-6763.	1.0	29
46	Structure-Guided Topographic Mapping and Mutagenesis to Elucidate Binding Sites for the Human Ether-a-Go-Go-Related Gene 1 Potassium Channel (KCNH2) Activator NS1643. Journal of Pharmacology and Experimental Therapeutics, 2012, 342, 441-452.	1.3	29
47	Modeling and protein engineering studies of active and inactive states of human dopamine D2 receptor (D2R) and investigation of drug/receptor interactions. Molecular Diversity, 2015, 19, 321-332.	2.1	29
48	Molecular modeling and in vitro approaches towards cholinesterase inhibitory effect of some natural xanthohumol, naringenin, and acyl phloroglucinol derivatives. Phytomedicine, 2018, 42, 25-33.	2.3	29
49	Synthesis, biological activity and multiscale molecular modeling studies for coumaryl-carboxamide derivatives as selective carbonic anhydrase IX inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 1042-1052.	2.5	28
50	Targeting the NF-Î¹B/IÎ¹BÎ± complex via fragment-based E-Pharmacophore virtual screening and binary QSAR models. Journal of Molecular Graphics and Modelling, 2019, 86, 264-277.	1.3	28
51	Near-physiological-temperature serial crystallography reveals conformations of SARS-CoV-2 main protease active site for improved drug repurposing. Structure, 2021, 29, 1382-1396.e6.	1.6	28
52	Proteinâ€“Protein Interactions: Inhibition of Mammalian Carbonic Anhydrases Iâ€“XV by the Murine Inhibitor of Carbonic Anhydrase and Other Members of the Transferrin Family. Journal of Medicinal Chemistry, 2012, 55, 5529-5535.	2.9	27
53	NS1643 Interacts around L529 of hERG to Alter Voltage Sensor Movement on the Path to Activation. Biophysical Journal, 2015, 108, 1400-1413.	0.2	27
54	Investigation of PDE5/PDE6 and PDE5/PDE11 selective potent tadalafil-like PDE5 inhibitors using combination of molecular modeling approaches, molecular fingerprint-based virtual screening protocols and structure-based pharmacophore development. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 311-330.	2.5	26

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55	Solubility profiles, hydration and desolvation of curcumin complexed with Î³-cyclodextrin and hydroxypropyl-Î³-cyclodextrin. Journal of Molecular Structure, 2017, 1134, 91-98.	1.8	26
56	In vitro and in silico approaches to appraise Polygonum maritimum L. as a source of innovative products with anti-ageing potential. Industrial Crops and Products, 2018, 111, 391-399.	2.5	26
57	AT1 antagonists: a patent review (2008 â€“ 2012). Expert Opinion on Therapeutic Patents, 2013, 23, 1483-1494.	2.4	25
58	Elucidation of Conformational States, Dynamics, and Mechanism of Binding in Human Î¼-Opioid Receptor Complexes. Journal of Chemical Information and Modeling, 2014, 54, 2294-2308.	2.5	25
59	Analysis of the Glutamate Agonist LY404,039 Binding to Nonstatic Dopamine Receptor D2 Dimer Structures and Consensus Docking. ACS Chemical Neuroscience, 2017, 8, 1404-1415.	1.7	23
60	Discovery of selective dengue virus inhibitors using combination of molecular fingerprint-based virtual screening protocols, structure-based pharmacophore model development, molecular dynamics simulations and in vitro studies. Journal of Molecular Graphics and Modelling, 2018, 79, 88-102.	1.3	23
61	Development of Small Molecule MEIS Inhibitors that modulate HSC activity. Scientific Reports, 2020, 10, 7994.	1.6	22
62	Virtual drug repurposing study against SARS-CoV-2 TMPRSS2 target. Turkish Journal of Biology, 2020, 44, 185-191.	2.1	22
63	In silicoinvestigation of PARP-1 catalytic domains inholoandapostates for the design of high-affinity PARP-1 inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 112-120.	2.5	21
64	Integration of multi-scale molecular modeling approaches with experiments for the in silico guided design and discovery of novel hERG-Neutral antihypertensive oxazalone and imidazolone derivatives and analysis of their potential restrictive effects on cell proliferation. European Journal of Medicinal Chemistry, 2018, 145, 273-290.	2.6	21
65	Novel tumor necrosis factor-Î± (TNF-Î±) inhibitors from small molecule library screening for their therapeutic activity profiles against rheumatoid arthritis using target-driven approaches and binary QSAR models. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2464-2476.	2.0	21
66	New nimesulide derivatives with amide/sulfonamide moieties: Selective COX-2 inhibition and antitumor effects. European Journal of Medicinal Chemistry, 2021, 221, 113566.	2.6	21
67	The neutralization effect of montelukast on SARS-CoV-2 is shown by multiscale in silico simulations and combined inÂvitro studies. Molecular Therapy, 2022, 30, 963-974.	3.7	21
68	Comparison of thermal effects of stilbenoid analogs in lipid bilayers using differential scanning calorimetry and molecular dynamics: correlation of thermal effects and topographical position with antioxidant activity. European Biophysics Journal, 2011, 40, 865-875.	1.2	20
69	Partial interdigitation of lipid bilayers. International Journal of Quantum Chemistry, 2011, 111, 1172-1183.	1.0	20
70	Leveraging NMR and X-ray Data of the Free Ligands to Build Better Drugs Targeting Angiotensin II Type 1 G-Protein Coupled Receptor. Current Medicinal Chemistry, 2015, 23, 36-59.	1.2	20
71	Drug repurposing studies of PARP inhibitors as a new therapy for inherited retinal degeneration. Cellular and Molecular Life Sciences, 2020, 77, 2199-2216.	2.4	20
72	Synthesis, molecular docking and molecular dynamics studies of novel tacrine-carbamate derivatives as potent cholinesterase inhibitors. Bioorganic Chemistry, 2021, 115, 105225.	2.0	19

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73	Structure-based design of hERG-neutral antihypertensive oxazalone and imidazolone derivatives. Journal of Molecular Graphics and Modelling, 2018, 79, 103-117.	1.3	18
74	In Silico Analysis of Bacteriocins from Lactic Acid Bacteria Against SARS-CoV-2. Probiotics and Antimicrobial Proteins, 2023, 15, 17-29.	1.9	18
75	Hostâ€"Guest Interactions between Candesartan and Its Prodrug Candesartan Cilexetil in Complex with 2-Hydroxypropyl-Î²-cyclodextrin: On the Biological Potency for Angiotensin II Antagonism. Molecular Pharmaceutics, 2019, 16, 1255-1271.	2.3	17
76	Current status of multiscale simulations on GPCRs. Current Opinion in Structural Biology, 2019, 55, 93-103.	2.6	17
77	Oligomerization and cooperativity in GPCRs from the perspective of the angiotensin AT1 and dopamine D2 receptors. Neuroscience Letters, 2019, 700, 30-37.	1.0	17
78	Design, Synthesis, and Molecular Modeling Studies of Novel Coumarin Carboxamide Derivatives as eEF-2K Inhibitors. Journal of Chemical Information and Modeling, 2020, 60, 1766-1778.	2.5	17
79	Integrating Ligand and Target-Driven Based Virtual Screening Approaches With in vitro Human Cell Line Models and Time-Resolved Fluorescence Resonance Energy Transfer Assay to Identify Novel Hit Compounds Against BCL-2. Frontiers in Chemistry, 2020, 8, 167.	1.8	17
80	Structural and dynamical properties of Bi3+ in water. Chemical Physics Letters, 2005, 406, 20-23.	1.2	16
81	An efficient synthesis of a rationally designed 1,5 disubstituted imidazole AT1 Angiotensin II receptor antagonist: reorientation of imidazole pharmacophore groups in losartan reserves high receptor affinity and confirms docking studies. Journal of Computer-Aided Molecular Design, 2010, 24, 749-758.	1.3	16
82	Structure Driven Design of Novel Human Ether-A-Go-Go-Related-Gene Channel (hERG1) Activators. PLoS ONE, 2014, 9, e105553.	1.1	16
83	Rehabilitating drug-induced long-QT promoters: In-silico design of hERG-neutral cisapride analogues with retained pharmacological activity. BMC Pharmacology & Toxicology, 2014, 15, 14.	1.0	16
84	Virtual screening of small molecules databases for discovery of novel PARP-1 inhibitors: combination of in silico and in vitro studies. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1899-1915.	2.0	16
85	Combined molecular modeling and cholinesterase inhibition studies on some natural and semisynthetic O-alkylcoumarin derivatives. Bioorganic Chemistry, 2019, 84, 355-362.	2.0	16
86	Molecular Simulations of Solved Co-crystallized X-Ray Structures Identify Action Mechanisms of PDEÎ´ Inhibitors. Biophysical Journal, 2015, 109, 1163-1168.	0.2	15
87	Biological Insights of the Dopaminergic Stabilizer ACR16 at the Binding Pocket of Dopamine D2 Receptor. ACS Chemical Neuroscience, 2017, 8, 826-836.	1.7	15
88	Kinetic and in silico analysis of thiazolidin-based inhibitors of Î±-carbonic anhydrase isoenzymes. Journal of Enzyme Inhibition and Medicinal Chemistry, 2013, 28, 370-374.	2.5	14
89	Kinetic andin silicostudies of hydroxy-based inhibitors of carbonic anhydrase isoforms I and II. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 31-37.	2.5	14
90	Atomistic molecular dynamics simulations of typical and atypical antipsychotic drugs at the dopamine D2 receptor (D2R) elucidates their inhibition mechanism. Journal of Biomolecular Structure and Dynamics, 2017, 35, 738-754.	2.0	14

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91	The effects of pollen, propolis, and caffeic acid phenethyl ester on tyrosine hydroxylase activity and total RNA levels in hypertensive rats caused by nitric oxide synthase inhibition: experimental, docking and molecular dynamic studies. Journal of Biomolecular Structure and Dynamics, 2018, 36, 609-620.	2.0	14
92	Identifying highly effective coumarin-based novel cholinesterase inhibitors by in silico and in vitro studies. Journal of Molecular Graphics and Modelling, 2022, 115, 108210.	1.3	14
93	The signaling pathway of dopamine D2 receptor (D2R) activation using normal mode analysis (NMA) and the construction of pharmacophore models for D2R ligands. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2040-2048.	2.0	13
94	Toward Understanding the Impact of Dimerization Interfaces in Angiotensin II Type 1 Receptor. Journal of Chemical Information and Modeling, 2019, 59, 4314-4327.	2.5	13
95	Formation of the inclusion complex of water soluble fluorescent calix[4]arene and naringenin: solubility, cytotoxic effect and molecular modeling studies. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3801-3813.	2.0	13
96	Screening of FDA approved drugs for finding potential inhibitors against Granzyme B as a potent drug-repurposing target. Journal of Molecular Graphics and Modelling, 2020, 95, 107462.	1.3	13
97	Comparative molecular dynamics simulations of the potent synthetic classical cannabinoid ligand AMG3 in solution and at binding site of the CB1 and CB2 receptors. Bioorganic and Medicinal Chemistry, 2008, 16, 7377-7387.	1.4	12
98	Synthesis of 1,4-bis(indolin-1-ylmethyl)benzene derivatives and their structureâ€“activity relationships for the interaction of human carbonic anhydrase isoforms I and II. Bioorganic and Medicinal Chemistry, 2013, 21, 1477-1482.	1.4	12
99	Biochemical changes induced by grape seed extract and low level laser therapy administration during intraoral wound healing in rat liver: an experimental and in silico study. Journal of Biomolecular Structure and Dynamics, 2018, 36, 993-1008.	2.0	12
100	Instant determination of the artemisinin from various Artemisia annua L. extracts by LCâ€ESIâ€MS/MS and their inâ€silico modelling and in vitro antiviral activity studies against SARSâ€CoVâ€2. Phytochemical Analysis, 2022, 33, 303-319.	1.2	12
101	Discovery of Klotho peptide antagonists against Wnt3 and Wnt3a target proteins using combination of protein engineering, proteinâ€“protein docking, peptide docking and molecular dynamics simulations. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 84-98.	2.5	11
102	Novel AChE and BChE inhibitors using combined virtual screening, text mining and in vitro binding assays. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3342-3358.	2.0	11
103	Identifying new piperazine-based PARP1 inhibitors using text mining and integrated molecular modeling approaches. Journal of Biomolecular Structure and Dynamics, 2021, 39, 681-690.	2.0	11
104	3D QSAR/CoMFA and CoMSIA Studies on Antileukemic Steroidal Esters Coupled with Conformationally Flexible Nitrogen Mustards. Journal of Chemical Information and Modeling, 2008, 48, 2254-2264.	2.5	10
105	Discovering novel carbonic anhydrase type IX (CA IX) inhibitors from seven million compounds using virtual screening andin vitroanalysis. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 31, 1-9.	2.5	10
106	Investigation of inhibition of human glucose 6-phosphate dehydrogenase by some 99mTc chelators byin silicoandin vitromethods. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 141-147.	2.5	9
107	First universal pharmacophore model for hERG1 K + channel activators: acthER. Journal of Molecular Graphics and Modelling, 2017, 74, 153-170.	1.3	9
108	Synthesis, anticholinesterase activity and molecular modeling studies of novel carvacrol-substituted amide derivatives. Journal of Biomolecular Structure and Dynamics, 2020, 38, 841-859.	2.0	9

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109	Screening of Clinically Approved and Investigation Drugs as Potential Inhibitors of SARSâ€CoVâ€2: A Combinedin silicoandinâ€...vitroStudy. Molecular Informatics, 2022, 41, e2100062.	1.4	9
110	Case Study of High-Throughput Drug Screening and Remote Data Collection for SARS-CoV-2 Main Protease by Using Serial Femtosecond X-ray Crystallography. Crystals, 2021, 11, 1579.	1.0	9
111	Molecular insights into the AT1 antagonism based on biophysical and in silico studies of telmisartan. Medicinal Chemistry Research, 2013, 22, 4842-4857.	1.1	8
112	Identification of novel serotonin reuptake inhibitors targeting central and allosteric binding sites: A virtual screening and molecular dynamics simulations study. Journal of Molecular Graphics and Modelling, 2017, 74, 193-202.	1.3	8
113	Proposing novel TNFÎ± direct inhibitor Scaffolds using fragment-docking based e-pharmacophore modeling and binary QSAR-based virtual screening protocols pipeline. Journal of Molecular Graphics and Modelling, 2018, 85, 111-121.	1.3	8
114	In silico characterization of adipokinetic hormone receptor and screening for pesticide candidates against stick insect, Carausius morosus. Journal of Molecular Graphics and Modelling, 2020, 101, 107720.	1.3	8
115	Transcription factor NF-ÎºB as target for SARS-CoV-2 drug discovery efforts using inflammation-based QSAR screening model. Journal of Molecular Graphics and Modelling, 2021, 108, 107968.	1.3	8
116	Integrated Binary QSAR-Driven Virtual Screening and In Vitro Studies for Finding Novel hMAO-B-Selective Inhibitors. Journal of Chemical Information and Modeling, 2020, 60, 4047-4055.	2.5	7
117	An Integrated in silico Approach and inâ€...vitro Study for the Discovery of Smallâ€Molecule USP7 Inhibitors as Potential Cancer Therapies. ChemMedChem, 2021, 16, 555-567.	1.6	7
118	Mechanism of K+Â/Na+selectivity in potassium channels from the perspective of the non-selective bacterial channel NaK. Channels, 2011, 5, 198-200.	1.5	6
119	Structural investigation of vesnarinone at the pore domains of open and open-inactivated states of hERG1 K + channel. Journal of Molecular Graphics and Modelling, 2017, 77, 399-412.	1.3	6
120	A QM proteinâ€“ligand investigation of antipsychotic drugs with the dopamine D2 Receptor (D2R). Journal of Biomolecular Structure and Dynamics, 2018, 36, 2668-2677.	2.0	6
121	Drug Reâ€positioning Studies for Novel HIVâ€1 Inhibitors Using Binary QSAR Models and Multiâ€targetâ€driven In Silico Studies. Molecular Informatics, 2021, 40, e2000012.	1.4	6
122	Bis benzothiophene Schiff bases: synthesis and in silico-guided biological activity studies. Turkish Journal of Chemistry, 2020, 44, 1164-1176.	0.5	6
123	Mechanistic insight into the impact of a bivalent ligand on the structure and dynamics of a GPCR oligomer. Computational and Structural Biotechnology Journal, 2022, 20, 925-936.	1.9	6
124	Design and synthesis of novel caffeic acid phenethyl ester (CAPE) derivatives and their biological activity studies in glioblastoma multiforme (GBM) cancer cell lines. Journal of Molecular Graphics and Modelling, 2022, 113, 108160.	1.3	6
125	Structural modeling of the N-terminal signalâ€“receiving domain of IÎºBÎ±. Frontiers in Molecular Biosciences, 2015, 2, 32.	1.6	5
126	Target-Driven Design of a Coumarinyl Chalcone Scaffold Based Novel EF2 Kinase Inhibitor Suppresses Breast Cancer Growth In Vivo. ACS Pharmacology and Translational Science, 2021, 4, 926-940.	2.5	5

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127	An effort to discover the preferred conformation of the potent AMG3 cannabinoid analog when reaching the active sites of the cannabinoid receptors. European Journal of Medicinal Chemistry, 2012, 47, 44-51.	2.6	4
128	Designing of multi-targeted molecules using combination of molecular screening and in silico drug cardiotoxicity prediction approaches. Journal of Molecular Graphics and Modelling, 2014, 50, 16-34.	1.3	4
129	Recent Developments of Carbonic Anhydrase Inhibitors as Potential Drugs. BioMed Research International, 2015, 2015, 1-2.	0.9	4
130	Mutated form (G52E) of inactive diphtheria toxin CRM197: molecular simulations clearly display effect of the mutation to NAD binding. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2462-2468.	2.0	4
131	Kinetic and docking studies of cytosolic/tumor-associated carbonic anhydrase isozymes I, II and IX with some hydroxylic compounds. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 1214-1220.	2.5	4
132	In vitro and in silico studies of nitrobenzamide derivatives as potential anti-neuroinflammatory agents. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4655-4668.	2.0	4
133	Proposing novel MDM2 inhibitors: Combined physicsâ€driven highâ€throughput virtual screening and in vitro studies. Chemical Biology and Drug Design, 2020, 96, 684-700.	1.5	4
134	Potent novel inhibitors against hepatitis C virus NS3 (HCV NS3 GT-3a) protease domain. Journal of Molecular Graphics and Modelling, 2020, 101, 107727.	1.3	4
135	Investigation of supramolecular interaction of quercetin with N,N-dimethylamine-functionalized p-sulfonated calix[4,8]arenes using molecular modeling and their in vitro cytotoxic response towards selected cancer cells. New Journal of Chemistry, 2021, 45, 18443-18452.	1.4	4
136	Structural and Functional Characterization of Allatostatin Receptor Type-C of Thaumetopoea pityocampa, a Potential Target for Next-Generation Pest Control Agents. Journal of Chemical Information and Modeling, 2021, 61, 715-728.	2.5	4
137	Novel inhibitors of eukaryotic elongation factor 2 kinase: In silico, synthesis and in vitro studies. Bioorganic Chemistry, 2021, 116, 105296.	2.0	4
138	Physics-driven identification of clinically approved and investigation drugs against human neutrophil serine protease 4 (NSP4): A virtual drug repurposing study. Journal of Molecular Graphics and Modelling, 2020, 101, 107744.	1.3	4
139	Evolutionary association of receptor-wide amino acids with G proteinâ€“coupling selectivity in aminergic GPCRs. Life Science Alliance, 2022, 5, e202201439.	1.3	4
140	In silico design of novel hERG-neutral sildenafil-like PDE5 inhibitors. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2830-2852.	2.0	3
141	Structural Investigation of the Dopamine-2 Receptor Agonist Bromocriptine Binding to Dimeric D2HighR and D2LowR States. Journal of Chemical Information and Modeling, 2018, 58, 826-836.	2.5	3
142	Structural modification of ellipticine derivatives with alkyl groups of varying length is influential on their effects on human DNA topoisomerase II: a combined experimental and computational study. Medicinal Chemistry Research, 2020, 29, 189-198.	1.1	3
143	Elucidation of interaction mechanism of hERG1 potassium channel with scorpion toxins BeKm-1 and BmTx3b. Journal of Molecular Graphics and Modelling, 2020, 96, 107504.	1.3	3
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